KENYATTA UNIVERSITY

UNIVERSITY EXAMINATIONS 2011/2012

INSTITUTE OF OPEN LEARNING – (IOL)

EXAMINATION FOR THE DEGREE OF BACHELOR OF EDUCATION (SCIENCE)

SPH 402: QUANTUM MECHANICS II

DATE: Wednesday, 14th December, 2011 TIME: 2.00 p.m. – 4.00 p.m.

INSTRUCTIONS: Attempt question **ONE** and any other **TWO** questions.

The following mathematical relations may be useful.

Laguerre polynomials, $L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x})$. Generalized Laguerre polynomials, $L_k^l(x) = -1^l \frac{d}{dx^l} L_{k+l}(x)$. Legendre polynomials $P_l(x) = \frac{d^l}{dx^l}(x^2-1)^l$. Associated Legendre $P_l^m = (1-x^2)^{|m|/2}\frac{d^m}{dx^m}P_l(x)$.

$\nabla = e_r \frac{\partial}{\partial r} + e_\theta \frac{\partial}{r\partial\theta} + e_\varphi \frac{1}{r sin\theta}\frac{\partial}{\partial\varphi}$ where e_r, e_θ and e_φ are unit vectors.

Q1. a) Quantum mechanics is a formulation of physics meant to describe sub atomic systems.

i. Identify the main parameter that is used for describing quantum systems. (3 Marks)

This parameter is obtained from an equation.

ii. Name and write down the equation from which the parameter is obtained. (4 Marks)

iii. What does the equation represent? Explain. (3 Marks)

iv. . Explain how is this parameter obtained from this equation. (4 Marks)

Dynamical variables are parameters that describe physical properties of a quantum system.

v. How are dynamical variables represented in quantum mechanics. (3 Marks)

vi. How are values of dynamical calculated? Explain. (4 Marks)

b) Hydrogen like atoms with single electrons are described as central field potential.

i. Explain why they are referred to as such. (3 Marks)

ii. Write down the fundamental equation for these quantum systems. (3 Marks)

iii. Propose how these equations can be solved. (Discuss only) (3 marks)

Q2. The wave function for an electron in a central field due to nuclear charge $+Ze$ can be written as follows,

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\Theta_{lm}(\theta)\Phi_m(\phi)$$

where $R_{nl}(r)$, $\Theta_{lm}(\theta)$ and $\Phi_m(\phi)$ are functions of r, radial distance and the angular variables θ and ϕ only respectively and n, l and m are quantum numbers.

i. Using the components of the wave function $R_{nl}(r)$, $\Theta_{lm}(\theta)$ and $\Phi_m(\phi)$, determine the wave function for the following wave function $\psi_{2,1,0}(r,\theta,\phi)$ i.e. expression for the quantum state $n = 2, l = 1, m = 0$ is given by

(10 Marks)

ii. Using this wave function or it's component write down the expression for the expectation value of a dynamical variable that depends only on the magnitude of the radial distance,r. (2 Marks)

iii. Hence determine the mean potential energy of an electron in the specified quantum state, i.e. $n = 2, l = 1, m = 0$. (8 Marks)

Q3.a) Show that by expressing the time-independent wave function $\psi(r,\theta,\phi)$ as a product of three independent functions of radial distance r, and the angular parameters θ and ϕ, the equation can be reduced to the equations written below,

$$\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR(r)}{dr}) + \left[-\frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2}\left[E + \frac{Ze^2}{r}\right]\right]R(r) = 0$$

and

$$\frac{1}{\sin(\theta)}\frac{d}{d\theta}(\sin(\theta)\frac{d\Theta}{d\theta}) + \left(l(l+1) - \frac{m^2}{\sin^2(\theta)}\right)\Theta = 0$$

where $m^2 = -\frac{1}{\Phi(\varphi)}\frac{d^2\Phi(\varphi)}{d\varphi^2}$ is a function of ϕ only and $R(r)$ and $\Theta(\theta)$ are functions of only r and θ respectively.

(10 marks)

b) Discuss the meanings of the additional term

$$-\frac{l(l+1)}{r^2}$$

in the equation for the radial function above. (4 marks)

c) Obtain explicit mathematical expressions for the functions $\Phi(\phi)$ (6 Marks)

Q4. a) List and discuss the meanings of all quantum numbers derivable from the Schrodinger's equation for the hydrogen atom. (8 marks)

b) Obtain the general equations for the components of angular momentum in Cartesian coordinates. (3 marks)

i) Obtain the equivalent expressions in quantum mechanics. (3 marks)

ii. Convert the equation for the component of angular momentum along the main (z) axis, l_z, to spherical polar coordinates. (4 marks)

iii. Explain why the component, l_z, is the only component whose eigenvalue can be non-zero if wave function is of the form $\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\varphi)$ and all terms have their usual meanings. (2 marks)

Q5. a) i. State Pauli's exclusion principle . (3 marks)

ii. Show how Pauli's exclusion principle can be used to explain the occupancy orbitals in multi-electron atoms and by extension the periodic table of atoms. (6 marks)

b) Discuss the general principles of Hartree's quantum theory of multi-electron atoms. (7 marks)

Explain why it is more acceptable than the Thomas-Fermi theory of many electron atoms. (4 marks)